What is claimed is:

1. A molecule or molecular complex comprising at least a portion of an *S. aureus* MurB or MurB-like FAD binding pocket, wherein the FAD binding pocket comprises the amino acids listed in Table 1, the FAD binding pocket being defined by a set of points having a root mean square deviation of less than about 1.7 Å from points representing the backbone atoms of said amino acids as represented by the structure coordinates listed in Figure 4.

2. The molecule or molecular complex of claim 1, wherein the FAD binding pocket comprises the amino acids listed in Table 2.

3. The molecule or molecular complex of claim 1, wherein the FAD binding pocket comprises the amino acids listed in Table 3.

4. A molecule or molecular complex comprising at least a portion of an *S. aureus* MurB or MurB-like substrate binding pocket, wherein the substrate binding pocket comprises amino acids listed in Table 4, the substrate binding pocket being defined by a set of points having a root mean square deviation of less than about 1.0 Å from points representing the backbone atoms of said amino acids as represented by the structure coordinates listed in Figure 4.

5. The molecule or molecular complex of claim 4, wherein the substrate binding pocket comprises the amino acids listed in Table 5.

6. The molecule or molecular complex of claim 4, wherein the substrate binding pocket comprises the amino acids listed in Table 6.

7. A molecule or molecular complex that is structurally homologous to an *S. aureus* MurB molecule or molecular complex, wherein the *S. aureus* MurB molecule or molecular complex is represented by at least a portion of the structure coordinates listed in Figure 4.

8. A scalable three dimensional configuration of points, at least a portion of said points derived from structure coordinates of at least a portion of an *S. aureus* MurB molecule or molecular complex listed in Figure 4 comprising at least one of a MurB or MurB-like FAD or substrate binding pocket.

9. A scalable three dimensional configuration of points, wherein substantially all of said points are derived from structure coordinates of an *S. aureus* MurB molecule or molecular complex listed in Figure 4.

10. The scalable three dimensional configuration of points of claim 8 wherein at least a portion of the points derived from the *S. aureus* MurB structure coordinates are derived from structure coordinates representing the locations of at least the backbone atoms of amino acids defining an *S. aureus* MurB FAD binding pocket, the FAD binding pocket comprising the amino acids listed in Table 1.

11. The scalable three dimensional configuration of points of claim 10 wherein the FAD binding pocket comprises the amino acids listed in Table 2.

12. The scalable three dimensional configuration of points of claim 10 wherein the FAD binding pocket comprises the amino acids listed in Table 3.

13. The scalable three dimensional configuration of points of claim 8 wherein at least a portion of the points derived from the *S. aureus* MurB structure coordinates are derived from structure coordinates representing the locations of at least the backbone atoms of amino acids defining an *S. aureus* MurB substrate binding pocket, the substrate binding pocket comprising the amino acids listed in Table 4.

14. The scalable three dimensional configuration of points of claim 13 wherein the substrate binding pocket comprises the amino acids listed in Table 5.

15. The scalable three dimensional configuration of points of claim 13 wherein the substrate binding pocket comprises the amino acids listed in Table 6.

16. The scalable three dimensional configuration of points of claim 8 displayed as a holographic image, a stereodiagram, a model or a computer-displayed image.

17. A scalable three dimensional configuration of points, at least a portion of the points derived from structure coordinates of at least a portion of a molecule or a molecular complex that is structurally homologous to an *S. aureus* MurB molecule or molecular complex and comprises at least one of an *S. aureus* MurB or MurB-like FAD or substrate binding pocket.

18. The scalable three-dimensional configuration of points of claim 17 displayed as a holographic image, a stereodiagram, a model or a computer-displayed image

19. A machine-readable data storage medium comprising a data storage material encoded with machine readable data which, when using a machine programmed with instructions for using said data, is capable of displaying a graphical three-dimensional representation of at least one molecule or molecular complex selected from the group consisting of:

(i) a molecule or molecular complex comprising at least a portion of an *S. aureus* MurB or MurB-like FAD binding pocket comprising the amino acids listed in Table 1, the FAD binding pocket defined by a set of points having a root mean square deviation of less than about 1.7 Å from points representing the backbone atoms of said amino acids as represented by structure coordinates listed in Figure 4; and

(ii) a molecule or molecular complex comprising at least a portion of an *S. aureus* MurB or MurB-like substrate binding pocket comprising the amino acids listed in Table 4, the substrate binding pocket defined by a set of points having a root mean square deviation of less than about 1.0 Å from points representing the backbone atoms of said amino acids as represented by structure coordinates listed in Figure 4; and

(iii) a molecule or molecular complex that is structurally homologous to an *S. aureus* MurB molecule or molecular complex, wherein the *S. aureus* MurB molecule or molecular complex is represented by at least a portion of the structure coordinates listed in Figure 4.

20. A machine-readable data storage medium comprising a data storage material encoded with a first set of machine readable data which, when combined with a second set of machine readable data, using a machine programmed with instructions for using said first set of data and said second set of data, can determine at least a portion of the structure coordinates corresponding to the second set of machine readable data, wherein said first set of data comprises a Fourier transform of at least a portion of the structural coordinates for *S. aureus* MurB listed in Figure 4; and said second set of data comprises an x-ray diffraction pattern of a molecule or molecular complex of unknown structure.

21. A method for obtaining structural information about a molecule or a molecular complex of unknown structure comprising:

crystallizing the molecule or molecular complex;

generating an x-ray diffraction pattern from the crystallized molecule or molecular complex;

applying at least a portion of the structure coordinates set forth Figure 4 to the x-ray diffraction pattern to generate a three-dimensional electron density map of at least a portion of the molecule or molecular complex whose structure is unknown.

22. A method for homology modeling an *S. aureus* MurB homolog comprising:

aligning the amino acid sequence of an *S. aureus* MurB homolog with an amino acid sequence of *S. aureus* MurB and incorporating the sequence of the *S. aureus* MurB homolog into a model of *S. aureus* MurB derived from structure coordinates set forth in Figure 4 to yield a preliminary model of the *S. aureus* MurB homolog;

subjecting the preliminary model to energy minimization to yield an energy minimized model;

remodeling regions of the energy minimized model where stereochemistry restraints are violated to yield a final model of the *S. aureus* MurB homolog.

23. A computer-assisted method for identifying an inhibitor of *S. aureus* MurB activity comprising:

supplying a computer modeling application with a set of structure coordinates of a molecule or molecular complex, the molecule or molecular complex comprising at least a portion of an *S. aureus* MurB or MurB-like FAD binding pocket, the FAD binding pocket comprising the amino acids listed in Table 1;

supplying the computer modeling application with a set of structure coordinates of a chemical entity; and

determining whether the chemical entity is an inhibitor expected to bind to or interfere with the molecule or molecular complex, wherein binding to or interfering with the molecule or molecular complex is indicative of potential inhibition of *S. aureus* MurB activity.

24. A computer-assisted method for identifying an inhibitor of *S. aureus* MurB activity comprising:

supplying a computer modeling application with a set of structure coordinates of a molecule or molecular complex, the molecule or molecular complex comprising at least a portion of an *S. aureus* MurB or MurB-like substrate binding pocket, the substrate binding pocket comprising the amino acids listed in Table 4;

supplying the computer modeling application with a set of structure coordinates of a chemical entity; and

determining whether the chemical entity is an inhibitor expected to bind to or interfere with the molecule or molecular complex, wherein binding to or interfering with the molecule or molecular complex is indicative of potential inhibition of *S. aureus* MurB activity.

25. The method of claim 23, wherein the FAD binding pocket comprises the amino acids listed in Table 1, the FAD binding pocket being defined by a set of points having a root mean square deviation of less than about 1.7 Å from points representing the backbone atoms of said amino acids as represented by structure coordinates listed in Figure 4.

26. The method of claim 24, wherein the substrate binding pocket comprises the amino acids listed in Table 4, the substrate binding pocket being defined by a set of points having a root mean square deviation of less than about 1.0 Å from points representing the backbone atoms of said amino acids as represented by structure coordinates listed in Figure 4.

27. The method of claim 23 or 24, wherein determining whether the chemical entity is an inhibitor expected to bind to or interfere with the molecule or molecular complex comprises performing a fitting operation between the chemical entity and a binding pocket of the molecule or molecular complex, followed by computationally analyzing the results of the fitting operation to quantify the association between, or the interference with, the chemical entity and the binding pocket.

28. The method of claim 23 or 24 further comprising screening a library of chemical entities.

29. A computer-assisted method for designing an inhibitor of *S. aureus* MurB activity comprising:

supplying a computer modeling application with a set of structure coordinates of a molecule or molecular complex, the molecule or molecular complex comprising at least a portion of an *S. aureus* MurB or MurB-like FAD binding pocket, the FAD binding pocket comprising the amino acids listed in Table 1;

supplying the computer modeling application with a set of structure coordinates for a chemical entity;

evaluating the potential binding or interfering interactions between the chemical entity and the FAD binding pocket of the molecule or molecular complex;

structurally modifying the chemical entity to yield a set of structure coordinates for a modified chemical entity; and

determining whether the modified chemical entity is an inhibitor expected to bind to or interfere with the molecule or molecular complex, wherein binding to the molecule or molecular complex is indicative of potential inhibition of *S. aureus* MurB activity.

30. A computer-assisted method for designing an inhibitor of *S. aureus* MurB activity comprising:

supplying a computer modeling application with a set of structure coordinates of a molecule or molecular complex, the molecule or molecular complex comprising at least a portion of an *S. aureus* MurB or MurB-like substrate binding pocket, the substrate binding pocket comprising the amino acids listed in Table 4;

supplying the computer modeling application with a set of structure coordinates for a chemical entity;

evaluating the potential binding or interfering interactions between the chemical entity and the substrate binding pocket of the molecule or molecular complex;

structurally modifying the chemical entity to yield a set of structure coordinates for a modified chemical entity; and

determining whether the modified chemical entity is an inhibitor expected to bind to or interfere with the molecule or molecular complex, wherein binding to the molecule or molecular complex is indicative of potential inhibition of *S. aureus* MurB activity.

31. The method of claim 29, wherein the FAD binding pocket comprises the amino acids listed in Table 1, the FAD binding pocket being defined by a set of points having a root mean square deviation of less than about 1.7 Å from points representing the backbone atoms of said amino acids as represented by structure coordinates listed in Figure 4.

32. The method of claim 30, wherein the substrate binding pocket comprises the amino acids listed in Table 4, the substrate binding pocket being defined by a set of points having a root mean square deviation of less than about 1.0 Å from points representing the backbone atoms of said amino acids as represented by structure coordinates listed in Figure 4.

33. The method of claim 29 or 30, wherein determining whether the modified chemical entity is an inhibitor expected to bind to or interfere with the molecule or molecular complex comprises performing a fitting operation between the chemical entity and a binding pocket of the molecule or molecular complex, followed by computationally analyzing the results of the fitting operation to quantify the association between or interference with the chemical entity and the binding pocket.

34. The method of claim 29 or 30, wherein the set of structure coordinates for the chemical entity is obtained from a chemical fragment library

35. A computer-assisted method for designing an inhibitor of *S. aureus* MurB activity *de novo* comprising:

supplying a computer modeling application with a set of structure coordinates of a molecule or molecular complex, the molecule or molecular complex comprising at least a portion of an *S. aureus* MurB or MurB-like FAD binding pocket, wherein the FAD binding pocket comprises the amino acids listed in Table 1;

computationally building a chemical entity represented by set of structure coordinates; and

determining whether the chemical entity is an inhibitor expected to bind to or interfere with the molecule or molecular complex, wherein binding to or interfering with the molecule or molecular complex is indicative of potential inhibition of *S. aureus* MurB activity.

36. A computer-assisted method for designing an inhibitor of *S. aureus* MurB activity *de novo* comprising:

supplying a computer modeling application with a set of structure coordinates of a molecule or molecular complex, the molecule or molecular complex comprising at least a portion of an *S. aureus* MurB substrate binding pocket, wherein the substrate binding pocket comprises the amino acids listed in Table 4;

computationally building a chemical entity represented by set of structure coordinates; and

determining whether the chemical entity is an inhibitor expected to bind to or interfere with the molecule or molecular complex, wherein binding to or interfering with the molecule or molecular complex is indicative of potential inhibition of *S. aureus* MurB activity.

37. The method of claim 35, wherein the FAD binding pocket comprises the amino acids listed in Table 1, the FAD binding pocket being defined by a set of points having a root mean square deviation of less than about 1.7 Å from points representing the backbone atoms of said amino acids as represented by structure coordinates listed in Figure 4.

38. The method of claim 36, wherein the substrate binding pocket comprises the amino acids listed in Table 4, the substrate binding pocket being defined by a set of points having a root mean square deviation of less than about 1.0 Å from points representing the backbone atoms of said amino acids as represented by structure coordinates listed in Figure 4.

39. The method of claim 35 or 36, wherein determining whether the chemical entity is an inhibitor expected to bind to or interfere with the molecule or

molecular complex comprises performing a fitting operation between the chemical entity and a binding pocket of the molecule or molecular complex, followed by computationally analyzing the results of the fitting operation to quantify the association between or interference with the chemical entity and the binding pocket.

40. The method of any of claims 23, 24, 29, 30, 35, or 36 further comprising supplying or synthesizing the potential inhibitor, then assaying the potential inhibitor to determine whether it inhibits *S. aureus* MurB activity.

41. A method for making an inhibitor of *S. aureus* MurB activity, the method comprising chemically or enzymatically synthesizing a chemical entity to yield an inhibitor of *S. aureus* MurB activity, the chemical entity having been identified during a computer-assisted process comprising supplying a computer modeling application with a set of structure coordinates of a molecule or molecular complex, the molecule or molecular complex comprising at least a portion of a *S. aureus* MurB or MurB-like FAD binding pocket or substrate binding pocket; supplying the computer modeling application with a set of structure coordinates of a chemical entity; and determining whether the chemical entity is expected to bind to or interfere with the molecule or molecular complex at a binding pocket, wherein binding to or interfering with the molecule or molecular complex is indicative of potential inhibition of *S. aureus* MurB activity.

42. A method for making an inhibitor of *S. aureus* MurB activity, the method comprising chemically or enzymatically synthesizing a chemical entity to yield an inhibitor of *S. aureus* MurB activity, the chemical entity having been designed during a computer-assisted process comprising supplying a computer modeling application with a set of structure coordinates of a molecule or molecular complex, the molecule or molecular complex comprising at least a portion of a *S. aureus* MurB or MurB-like FAD binding pocket or substrate binding pocket; supplying the computer modeling application with a set of structure coordinates for a chemical entity; evaluating the potential binding

interactions between the chemical entity and a binding pocket of the molecule or molecular complex; structurally modifying the chemical entity to yield a set of structure coordinates for a modified chemical entity; and determining whether the chemical entity is expected to bind to or interfere with the molecule or molecular complex at the binding pocket, wherein binding to or interfering with the molecule or molecular complex is indicative of potential inhibition of *S. aureus* MurB activity.

43. A method for making an inhibitor of *S. aureus* MurB activity, the method comprising chemically or enzymatically synthesizing a chemical entity to yield an inhibitor of *S. aureus* MurB activity, the chemical entity having been designed during a computer-assisted process comprising supplying a computer modeling application with a set of structure coordinates of a molecule or molecular complex, the molecule or molecular complex comprising at least a portion of a *S. aureus* MurB or MurB-like FAD binding pocket or substrate binding pocket; computationally building a chemical entity represented by set of structure coordinates; and determining whether the chemical entity is expected to bind to or interfere with the molecule or molecular complex at a binding pocket, wherein binding to or interfering with the molecule or molecular complex is indicative of potential inhibition of *S. aureus* MurB activity.

44. An inhibitor of *S. aureus* MurB activity identified, designed or made according to the method of any of the claims 23, 24, 29, 30, 35, 36, 41, 42, or 43.

45. A composition comprising an inhibitor of *S. aureus* MurB activity identified, designed or made according to the method of any of claims 23, 24, 29, 30, 35, 36, 41, 42, or 43.

46. A pharmaceutical composition comprising an inhibitor of *S. aureus* MurB activity identified or designed according to the method of any of claims 23, 24, 29, 30, 35, 36, 41, 42, or 43 or a salt thereof, and pharmaceutically acceptable carrier.

47. A method for crystallizing an *S. aureus* MurB molecule or molecular complex comprising:

preparing purified *S. aureus* MurB at a concentration of about 1 mg/ml to about 50 mg/ml; and

crystallizing *S. aureus* MurB from a solution comprising about 1 wt. % to about 50 wt. % PEG, 0 wt. % to about 40 wt. % DMSO, about 100 mM to about 1 M ammonium or lithium sulfate, about 0 mM to about 20 mM 2-mercaptoethanol, about 0.005 mM to about 40 mM EP-UDPGlcNAc, and buffered to a pH of about 5 to about 8.

48. A crystal of *S. aureus* MurB.

49. The crystal of claim 48 having the trigonal space group symmetry $I2_13$.

50. The crystal of claim 48 comprising a unit cell having dimensions a = b = c = 178.9 ± 20 Å, and $\alpha = \beta = \gamma = 90°$.

51. The crystal of claim 48 comprising atoms arranged in a spatial relationship represented by the structure coordinates listed in Figure 4.

52. The crystal of claim 48 wherein MurB has amino acid sequence SEQ ID NO:1.

53. The crystal of claim 48 wherein MurB amino acid sequence SEQ ID NO:1, except that at least one methionine is replaced with selenomethionine.